Kondo resonance for orbitally degenerate systems

A. K. Zhuravlev,[1,2] V. Yu. Irkhin,[1,3] M. I. Katsnelson,[3,2] and A. I. Lichtenstein[2,4]

[1] *Institute of Metal Physics, 620219 Ekaterinburg, Russia*
[2] *University of Nijmegen, NL 6525 ED Nijmegen, The Netherlands*
[3] *Department of Physics, Uppsala University, Box 530, SE-751 21 Uppsala, Sweden*
[4] *Institute of Theoretical Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany*

Formation of the Kondo state in general two-band Anderson model has been investigated within the numerical renormalization group (NRG) calculations. The Abrikosov-Suhl resonance is essentially asymmetric for the model with one electron per impurity (quarter filling case) in contrast with the one-band case. An external magnetic (pseudo-magnetic) field breaking spin (orbital) degeneracy leads to asymmetric splitting and essential broadening of the many-body resonance. Unlike the standard Anderson model, the "spin up" Kondo peak is pinned against the Fermi level, but not suppressed by magnetic field.

PACS numbers: 71.10.Fd 71.27.+a 71.28.+d

The Kondo problem is one of most fascinating and important issues in condensed matter theory. It was originally formulated for explanation of the resistivity minimum in metallic alloys [1] due to the scattering of conduction electrons by a magnetic impurity, and later generalized to various cases. The Kondo effect turns out to be a key phenomenon of the heavy fermion behavior [2], anomalous electronic properties of metallic glasses at low temperatures [3], quantum dots [4], and many other correlated electron problems. One of the main results of this theory is the formation of a resonance with small energy scale (so-called, the Kondo temperature T_K) near the Fermi energy due to the scattering of conduction electrons by local quantum systems with internal degrees of freedom. Originally this resonance (usually called the Kondo, or Abrikosov-Suhl resonance; for a review, see Ref. 2) could be experimentally investigated only indirectly, through the temperature dependence of thermodynamic and transport properties of metals. However, novel tunneling spectroscopy, in particular scanning tunneling microscopy (STM), is now able to directly visualize the Kondo resonance [5, 6, 7]. At the same time, theoretical investigation of the spectral density for Kondo systems is a much more complicated problem than the calculation of thermodynamic properties. Indeed, in the latter case exact analytical results can be derived by the Bethe Ansatz [8], whereas the electron density of states is considered mainly by some approximate methods or numerically, see, e.g., Refs. 9, 10, 11, 12, 13, 14, 15, 16. The splitting of the Kondo resonance by external magnetic field was investigated by Bethe Ansatz for the *s-d* exchange model [17]. These results can be used to verify different approximate schemes demonstrating some difficulties, for example, with the well-known non-crossing approximation (NCA) [10].

Generally speaking, we have now a complete and satisfactory theory of the Kondo resonance for the prototype case of purely spin scattering. On the other hand, the information about the systems with orbital degrees of freedom is still insufficient. A so-called "orbital Kondo resonance" has been considered theoretically, for atomic two-level systems in metallic glasses, for quadrupolar degrees of freedom in some uranium-based compounds [3], for high-temperature superconductors [18], and for double quantum dot systems [19]. Recently the phase diagram of the Anderson model with orbital degrees of freedom has been investigated by the numerical renormalization group (NRG) method [20]. Spin (pseudospin) susceptibility for the double quantum dot model has been investigated by this technique in Ref. 19. However, electron spectral density has not been calculated. It is worthwhile to note that investigation of dynamical properties for effective impurity models is of the crucial importance for the dynamical mean-field theory (DMFT) approach, in particular, to describe the metal-insulator transition and related phenomena [21]. For one-band case the NRG method was applied to DMFT problem in Ref. 22.

Direct observation of the orbital Kondo resonance on Cr(001) surface by the STM measurements [7], as well as a relevance for multiple quantum dot systems [19], makes the issue about the shape of the Kondo resonance and about effects of "pseudomagnetic" field which breaks the orbital degeneracy especially actual. Here we investigate the problem of orbital Kondo resonance by the NRG approach [23]. We shall demonstrate that in the "orbital" Kondo case the resonance has an essential asymmetry with respect to the Fermi energy, in qualitative agreement with the experimental observations [7].

We start from the two-band Anderson impurity model with the spin and orbital rotationally invariant Hamiltonian [24]

$$H = \sum_{\mathbf{k}a\sigma} \left[\varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}a\sigma} c_{\mathbf{k}a\sigma} + V\left(f^{\dagger}_{a\sigma} c_{\mathbf{k}a\sigma} + c^{\dagger}_{\mathbf{k}a\sigma} f_{a\sigma} \right) \right] + H_{\mathrm{imp}} \tag{1}$$

where

$$H_{\rm imp} = \sum_{a\sigma}\Big(\varepsilon_{\rm f} - \frac{h\sigma}{2}\Big) f^{\dagger}_{a\sigma} f_{a\sigma} + \frac{U+J}{2}\sum_{a\sigma} n_{a\sigma} n_{a-\sigma} + \sum_{a\neq b,\sigma}\left(\frac{U}{2} n_{a\sigma} n_{b-\sigma} + \frac{U-J}{2} n_{a\sigma} n_{b\sigma} - \frac{J}{2} f^{\dagger}_{a\sigma} f_{a-\sigma} f^{\dagger}_{b-\sigma} f_{b\sigma}\right)$$

Here $a, b = 1{,}2$ and $\sigma = \uparrow, \downarrow$ are orbital and spin indices, correspondingly, $c^{\dagger}_{\mathbf{k}a\sigma}(c_{\mathbf{k}a\sigma})$ denote the creation (annihilation) operators for a-orbital states with spin σ and energy $\varepsilon_{\mathbf{k}}$ (we take the rectangle band with half width $D = 2$), $f^{\dagger}_{a\sigma}(f_{a\sigma})$ those for impurity states of a-orbital with spin σ and energy $\varepsilon_{\rm f}$, $n_{a\sigma} = f^{\dagger}_{a\sigma} f_{a\sigma}$, h is magnetic field. Since the spin and orbital degrees of freedom are symmetric in the Hamiltonian, h may be a pseudomagnetic field (e.g., for the orbital Kondo effect on Cr(001) surface where the potential of the atomic step edge breaks the exact degeneracy between d_{xz} and d_{yz} states [7]). The Coulomb interaction and exchange parameter at the impurity site are U and J, and two electron subsystems are coupled via a hybridization parameter V. Note that in solids the orbital moment conservation is not an exact property and therefore some additional terms in the Hamiltonian may appear [25]. However, we omit them since the problem turns out to be numerically very cumbersome even for the rotationally invariant Hamiltonian.

To calculate the spectral properties of impurity we use the NRG technique which is described in details in Refs. 2, 11, 23, 26. Here we emphasize the new aspects for multi-orbital Anderson model.

As usually, we start from the solution of the isolated impurity problem. As an initial step of the RG procedure, we add the first conduction electron site, diagonalize the Hamiltonian matrix for this Hilbert space, and thus obtain new eigenstates. Then such a procedure should be repeated until reaching a fixed point. Dimension of the Hilbert space within one NRG-iteration increases by factor 16 instead of 4 for the one-band case. By using an appropriate symmetry of the problem we were able to find the whole spectrum for the Hilbert space with the dimensionality of 48000 states, which gives a possibility to keep at each step about 3000 states [27].

Due to the NRG discretization scheme, the electron spectral function

$$\rho_f(\omega) = -\frac{1}{\pi}{\rm Im}G(\omega + i0)\ , \qquad G(z) = \langle\langle f_{a\sigma} | f^{\dagger}_{a\sigma}\rangle\rangle_z$$

is given by a set of δ-functional peaks at the frequencies ω_n. Standard NRG practice consists of the Gaussian broadening of the spectral function on a logarithmic scale [11]. Since the point $\omega = 0$ plays special role in such a scheme, we used more conventional Gaussian broadening

$$\delta(\omega - \omega_n) \to \frac{1}{b_L\sqrt{\pi}} \exp\left[-\frac{(\omega-\omega_n)^2}{b_L^2}\right], \qquad (2)$$

smearing being changed depending on the iteration number L, namely, $b_{L+2} = b_L/\Lambda$ (where the NRG cutoff parameter $\Lambda = 2$ have been used).

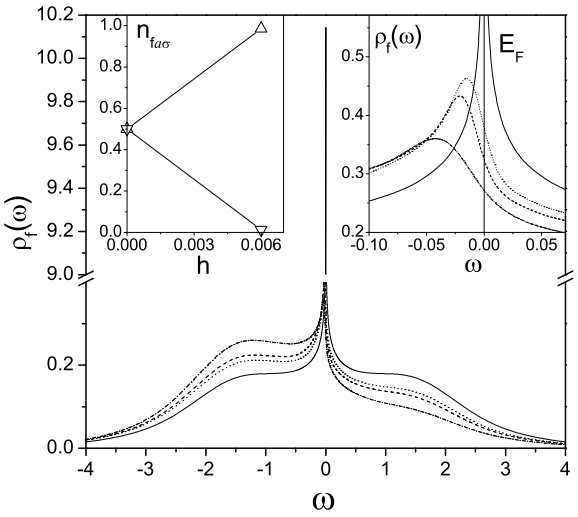

FIG. 1: The density of states for the half-filled case, $\varepsilon_{\rm f} = -3, V = 0.2, U = 2, J = 0, h = 0$ (solid) and symmetric splitting (only the spin-up DOS) in the magnetic field $h = 0.006$ (dot), $h = 0.01$ (dash) and $h = 0.02$ (dash-dot). Occupation number per orbital and spin are shown in the left insert (total $n_f = 2$). Density of states at the Fermi level according to the Friedel sum rule (3) is $\rho_f(0) = 10.13$. Right insert shows the DOS in the vicinity of the Fermi level.

The Kondo regime corresponds to the case where $|\varepsilon_{\rm f}| \gtrsim 2\Gamma$ [12], $\Gamma = \pi V^2\rho$ being the one-particle resonance width for the localized electrons, ρ is the bare DOS of conduction electrons at E_F. The density of states for the half-filled case ($n_f = 2$) and for almost quarter-filled case ($n_f \approx 1$) are shown in Figs. 1 and 2, respectively. Although the Hund interaction J was estimated to have considerable value [7], this quantity is irrelevant for the quarter-filled case; our RG calculations confirmed that J does not influence essentially the results (see insert in Fig. 2). The main difference of the NRG results obtained here with those for the nondegenerate Anderson model is that the Kondo peak is not centered at the Fermi energy $E_F = 0$. An explanation of this deviation is given by the Friedel sum rule for the phase shifts η_l: $2(2l{+}1)\eta_l/\pi = n_f$ [28], $2l+1$ being the number of orbital channels and n_f the total number of localized electrons. It is important that due to locality of the self-energy the value of $\rho_f(0)$ does not change in comparison with the non-interacting model ($U = 0$) and is equal to

$$\rho_f(0) = \frac{1}{\pi\Gamma}\sin^2\left(\frac{\pi n_f}{N}\right), \qquad (3)$$

where N is the degeneracy factor [29]. For the standard $SU(2)$ Kondo model for $S = 1/2$, as well as for a degenerate half-filled model, the phase shift at E_F is close to $\pi/2$ which means the strongest possible scattering at the

top of the resonance peak. In this case the asymmetry of the Kondo resonance with respect to E_F should be very weak even for the nonsymmetric Anderson model, in agreement with recent computational results [16], and with our Fig. 1. Thus the large value of electronic effective mass and linear specific heat is owing to renormalization of the residue of the electron Green's function,

$$Z = \left(1 - \left.\frac{\partial \mathrm{Re}\Sigma(E)}{\partial E}\right|_{E=E_F}\right)^{-1} \qquad (4)$$

On the other hand, for $N > 2$ and $n_f \approx 1$ the top of the f-electron peak shifts above E_F [2]. In particular, in the $SU(N)$ Anderson model (or in the equivalent Coqublin-Schrieffer model) with infinitely large N [9, 10] the high peak lies *completely* above the Fermi level, being shifted by the value of the order of T_K (note that in the limit $N \to \infty$ this is just a delta-like peak). NRG calculations for $SU(N)$ Anderson model [11] give qualitatively similar results. However, the values of $\rho_f(0)$ calculated in Ref. [11] turn out to be by about 30% smaller than given by Eq.(3), probably, due to insufficient accuracy. Our results for double-degenerate model give $\rho_f(0)$ in the perfect agreement with the Friedel sum rule (see captions to Fig. 1).

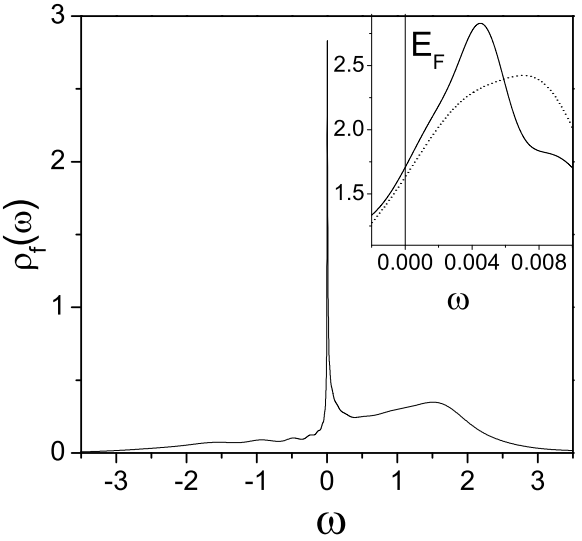

FIG. 2: The density of states for the almost quarter-filled case for $\varepsilon_f = -1, U = 2, J = 0, V = 0.35$. Occupation number per orbital and spin is 0.258 (total $n_f = 1.032$). Insert shows the DOS in the vicinity of the Fermi level; the dash line corresponds to the case of non-zero exchange parameter $J = 0.2$.

The NRG calculations with the external magnetic field h were also performed. Since we are interested only in a small energy region, shortcomings of the NRG scheme, which occur in the presence of magnetic field at large excitation energies ω [30], are not important here. There are several qualitatively different regimes of magnetic splitting in the double-degenerate Anderson model:

(i) a half-filled case where $n_f = 2$ due to electron-hole symmetry even in the presence of external magnetic field. The usual symmetrical splitting takes place, the Kondo peaks becomes low and broad (Fig. 1), similar to the behavior in the non-degenerate symmetric Anderson model [16].

(ii) a nearly quarter-filled case: $n_f \approx 1$. The splitting of the Kondo peak is asymmetric. One can see from Fig. 3 that the upper "spin down" peak becomes low and broad, as well as in the symmetric case. At the same time, the lower "spin up" peak is not suppressed (as in the standard Kondo model), but tends to the Fermi level and becomes more high (however, the situation changes with decreasing V: the height and area of spin-up peak decreases considerably in strong magnetic field). The density of states at E_F remains high up to very strong fields, so that the partial f-occupation numbers depend strongly on h. For very strong fields the peak corresponding to spin down states is completely suppressed ($n_{fa\downarrow} \to 0$), and only orbital Kondo resonance between spin up states survives since $n_{fa\uparrow} \to 1/2$, in contrast with the case (i) where $n_{fa\uparrow} \to 1$.

(iii) the intermediate valence regime (n_f is essentially non-integer). Instead of the three-peak structure characteristic for the Kondo regime, we have one peak which is split in magnetic field (Fig. 4).

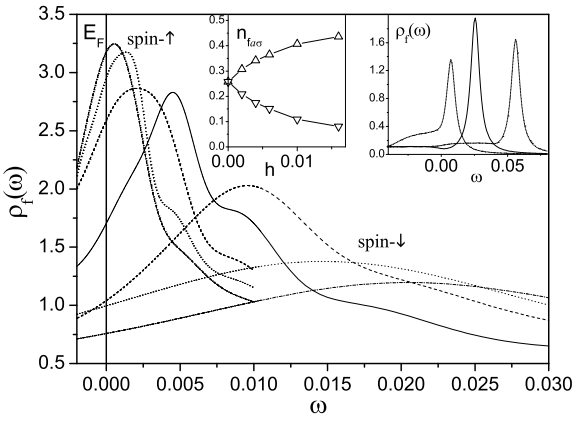

FIG. 3: The effect of the magnetic field on the density of states for the same model parameters as in Fig. 2. The magnetic field values are $h = 0$ (solid), 0.006 (dash), 0.01 (dot), 0.016 (dash-dot). The left insert displays the dependence of occupation numbers on the magnetic field; the right one shows the result of the approximation (5) for $\varepsilon_f = -1, U = \infty, J = 0, V = 0.56, h = 0$ (solid) and $h = 0.04$ (dot), the smearing of the logarithm with $\delta = 0.004$ being introduced. The value of V is increased in comparison with the finite-U case to obtain a comparable value of the Kondo temperature.

The NRG method can provide a detailed information about the Kondo resonance in the two-band Anderson model. For larger number of orbitals, numerical calcula-

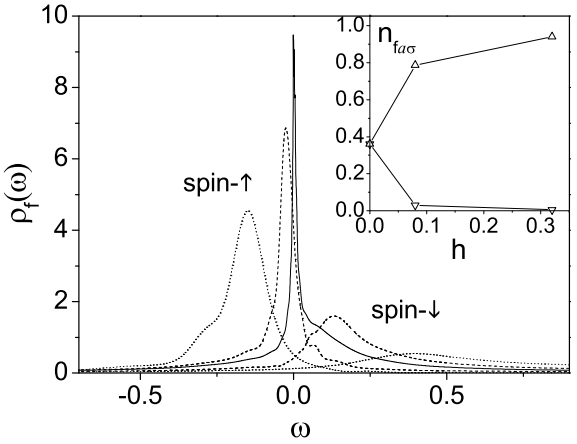

FIG. 4: The effect of the magnetic field on the density of states for $\varepsilon_{\rm f} = -2, U = 2, J = 0, V = 0.2$. The magnetic field values are $h = 0$ (solid), 0.08 (dash), 0.32 (dot). The insert shows the spin-occupation number as function of magnetic fields.

tions become impractical for a reliable treatment of the Kondo problem. To understand qualitatively the behavior of the multiband Kondo system in magnetic field, we consider a simple degenerate Anderson model with $U = \infty$ where the peak lies also above the Fermi level [10]. The Hamiltonian reads

$$\mathcal{H} = \sum_{\mathbf{k}m} t_{\mathbf{k}} c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \sum_m (\varepsilon_{\rm f} - h_m) f^\dagger_m f_m + V \sum_{\mathbf{k}m} \left[c^\dagger_{\mathbf{k}m} f_m + h.c. \right]$$

where $f^\dagger_m = |m\rangle\langle 0|$ are the Hubbard's X-operators; the model (1) corresponds to $m = a\sigma$ and $h_{a\uparrow} = h/2$, $h_{a\downarrow} = -h/2$. Using the second-order perturbation theory for X-operators [31] one can obtain (cf. also Refs. [9, 10])

$$\langle\langle f_m | f^\dagger_m \rangle\rangle_E = \langle n_0 + n_m \rangle \big[E - \varepsilon_{\rm f} + h_m - \rho V^2 \sum_{m' \neq m} \ln \frac{D}{E + h_m - h_{m'}} \big]^{-1} \qquad (5)$$

This very simple approximation gives reasonable *qualitative* agreement with the numerically accurate NRG results (see right insert in Fig. 3). It can be used for interpretations of the computational results. For example, according to Eq.(5), the spin up peak does not intersect the Fermi level with increasing magnetic field (at least, at not too small V). Indeed, the logarithmic divergence of the self-energy exists in our orbitally-degenerate model, the contribution from the transitions between the degenerate states being not cut at h.

To conclude, we have considered peculiarities of the Kondo resonance in the orbital-degenerate case by a numerical renormalization group technique. A possibility to calculate the spectral properties for degenerate Anderson impurity model is demonstrated, which gives a chance to extend the applicability region of the NRG scheme in the DMFT approach beyond the one-band case. Our version of the NRG can describe accurately the case where the Kondo peak is shifted from the Fermi energy, which is a generic case of multiband impurity model. The new features of the orbital-degenerate model are related with a fact, that the Kondo resonance is not suppressed by external magnetic (or pseudomagnetic) field, its splitting being essentially asymmetric.

The work was supported by the Netherlands Organization for Scientific Research (NWO project 047.016.005) and the Russian Academy of Sciences, grant No.NSh-747.2003.2.

[1] J. Kondo, Prog. Theor. Phys. **32**, 37 (1964).
[2] A. C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge University Press, Cambridge, 1993.
[3] D. L. Cox and A. Zawadowski, Adv. Phys. **47**, 599 (1998).
[4] L. Kouwenhoven and L. I. Glazman, Physics Worlds, January 2001, p.33; I. L. Aleiner et al, Phys. Rep. **358**, 309 (2002).
[5] V. Madhavan et al, Science **280**, 567 (1998); J. Li et al, Phys. Rev. Lett. **80**, 2893 (1998).
[6] H. C. Manoharan et al, Nature **403**, 512 (2000).
[7] O. Yu. Kolesnychenko et al, Nature **415**, 507 (2002).
[8] A. M.Tsvelick and P. B. Wiegmann, Adv. Phys. **32**, 745 (1983); N. Andrei et al, Rev. Mod. Phys. **55**, 331 (1983).
[9] O. Gunnarsson and K. Schönhammer, Phys. Rev. B **28**, 4315 (1983).
[10] N. E. Bickers, Rev. Mod. Phys. **59**, 845 (1987).
[11] O. Sakai et al, J. Phys. Soc. Japan **58**, 3666 (1989).
[12] T. A. Costi et al, Phys. Rev. B **53**, 1850 (1996).
[13] K. Haule et al, Phys. Rev. B **64**, 155111 (2001).
[14] A. Rosch et al, Phys. Rev. B **68**, 014430 (2003).
[15] D. E. Logan and N. L. Dickens, J. Phys.: Cond. Mat.**13**, 9713 (2001).
[16] M. T. Glossop and D. E. Logan, J. Phys.: Cond. Mat.**14**, 6737 (2002).
[17] J. E. Moore and X.-G. Wen, Phys. Rev. Lett. **85**, 1722 (2000).
[18] V. Yu. Irkhin et al, Europhys. Lett. **15**, 649 (1991).
[19] L. Borda et al, Phys. Rev. Lett. **90**, 026602 (2003).
[20] M. Fabrizio et al, Phys. Rev. Lett. **91**, 246402 (2003).
[21] A. Georges et al, Rev. Mod. Phys. **68**, 13 (1996).
[22] R. Bulla et al, J. Phys.: Cond. Mat.**10**, 8365 (1998).
[23] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975); H. R. Krishna-murthy et al, Phys. Rev. B **21**, 1003 (1980); ibid **21**, 1044 (1980).
[24] L. Dworin and A. Narath, Phys. Rev. Lett. **25**, 1287 (1970).
[25] P. Noziéres and A. Blandin, J. de Physique **41**, 193 (1980).
[26] T. A. Costi et al, J. Phys.: Cond. Mat. **6**, 2519 (1994).
[27] Details of multiband NRG calculations will be published elsewhere.
[28] D. C. Langreth, Phys. Rev. **150**, 516 (1966).
[29] G. Grüner and A. Zawadowski, Rep. Prog. Phys. **37**, 1497 (1974).
[30] W. Hofstetter, Phys. Rev. Lett. **85**, 1508 (2000).
[31] V. Yu. Irkhin and Yu. P. Irkhin, JETP **80**, 334 (1995).